



Numerical modeling of compression ignition engine: A review

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ABSTRACT

Diesel engine modeling draws the greater attention due to its higher efficiency as compared to spark ignition (SI) engine. Still it is very challenging job to model diesel engine due to its complex combustion phenomena. The focus of the present study is to review the different available model used for modeling of CI engines. The modeling of CI engine is divided into single zone, multizone and multi-dimensional model. Which further subdivided in many submodel i.e. heat transfer, ignition delay period, droplet evaporation, intake and exhaust flow, chemical kinematics and soot formation model. A comparative study has also been carried out with experimental validation to show the compatibility with different modeling approach. Some optimum mathematical input parameter has been suggested by the analysis of different modeling approach to minimize the NO_x emission and soot formation to make diesel engine more eco-friendly.

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1. Introduction

One of the major pollution contributors in today's environment is the internal combustion (IC) engine which has been either spark or compression ignition (CI) engine. Due to scarcity of

the crude oil and its high rising price makes a challenging job for the engine manufacturers to manufacture or model less polluting and more efficient engine in order to meet its future demands [1,2].

Engine simulation has been extensively used to improve the engine performance. Compression ignition direct injection (CIDI) diesel engines have been widely used in heavy-duty vehicle, marine transportation and now have been increasingly being used in light duty vehicles, particularly in Europe and Japan [3].

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Nomenclature

A	pre-exponential factor
A_n	minimum area of nozzle (m)
A_c	cylinder area (m ²)
A_e	effective flow area (m ²)
a_1	empirical constant
C_d	coefficient of discharge
D	cylinder diameter (m)
E_A	activation energy
F_S	geometric circulation area of inlet (m ²)
K	adiabatic exponent of working fluid in a cylinder
k_i	rate constant (cm ³ /mol-s)
K_s	adiabatic exponent of working fluid before inlet valve
m	mass flow rate (kg/s)
m_s	mass of soot
m_{fg}	masses of vaporized fuel
m_{sf}	rates of soot formation
P	cylinder pressure (bar)
P_r	preparation rate (kg/Crank angle)
P_a	pressure at the inlet (bar)
P_m	motored pressure (bar)
P_1	upstream and stagnation pressures (bar)
P_2	downstream stagnation pressures (bar)
p_m	average mean pressure
P_{O_2}	partial pressure of oxygen
P_S	pressure of working fluid before inlet valve
P_r	pressure of working fluid after outlet valve

R	universal gas constant (J mol ⁻¹ K ⁻¹)
Re	Reynolds number
T	temperature inside the cylinder (K)
T_w	temperature of the cylinder wall (K)
T_a	activation temperature (K)
T_g	temperature of gas (K)
up	piston speed (m/s)
V	volume of the cylinder (m ³)

Greek

Δp	pressure drop (bar)
$d\phi$	change in crank angle (degree)
σ	surface tension (N/m)
μ_s	inlet valve flow coefficient
ρ_a	density of liquid (kg/m ³)
θ	spray angle (rad)
γ	ratio of the specific heats
λ_g	gas thermal conductivity
μ_a	viscosity of the ambient gas

Subscripts

<i>inj</i>	injection of fuel
<i>soc</i>	start of combustion
<i>f</i>	fuel

Experimental work which is aimed at fuel economy and low pollutants emission for IC engine requires change in input parameter which is highly demanding in terms of money and time. So, in order to overcome this drawback, an alternative simulation of engine performance with the help of mathematical model and powerful digital computers lowers the cost and time. In these simulation models, the effect of various design structures like design of combustion chamber input parameters (intake pressure, injection timing, etc.) and operation changes (compression ratio, speed, etc.) can be estimated in fast and non-expensive way provided that main mechanism are recognized and modeled perfectly to meet the experimental results [4,5].

In case of single zone model cylinder temperature, pressure and mass can be obtained from ordinary differential equations. These models do not take into account the air entrainment, vaporization of fuel droplet and spatial variation of mixture composition and temperature. Single zone models are advantageous also because of their simplicity and their wide usage along with empirical data within the engine industry to make design decisions. The measured pressure rise in an engine is used to tune the model and helps in calculating the rate of heat release from the engine cylinder [6].

For the accurate prediction and study the behavior of exhaust emission pollutants, forced the researchers to develop two zone combustion models [7–10]. It provides more accurate result as compared to single zone. Multizone model overcomes the drawbacks of single zone model taking into account both the spatial as well as temporal variation of temperature and concentration, where the detailed analysis of fuel–air distribution which permits calculation of exhaust gas composition within the reasonable accuracy [11–14]. Multizone models separate the fuel spray into a large, finite number of zones. Zones are small packets of fuel that move through the combustion chamber. A second type of multizone model follows the

development of equivalence ratio zones surrounding a central liquid core.

In multi-dimensional model, the instantaneous conservation time average equation of mass, momentum, energy has been taken into calculation. Stochastic as well as computational fluid dynamics (CFD) model are introduced to see the effect of gas phase turbulence on the liquid droplets. However, the effect of droplets on turbulence in many parts has also been ignored. Cylinder is considered to be divided into number of zones and behavior of each individual zone being studied.

In this review paper different modeling approach and their comparison along theoretical and experimental results was reviewed. It also investigates the engine parameter and their effect on the performance of the engine major pollutant such as NO_x and soot formation. Classification of various diesel engine models has been presented in Fig. 1.

2. Engine submodels

Submodels included in the study of the smallest region inside the engine cylinder which helps in proper understanding of the actual phenomena of the engine. It includes the different engine submodels which also help to study complex behavior of the combustion.

2.1. Intake and exhaust manifold submodel

Intake and exhaust manifold submodel deals with the mass flow rate inside the cylinder either the air entering during the intake stroke, mass of fuel during the compression stroke and the amount of gases flow through the exhaust stroke. The timing and rate of fuel injection into the chamber affects the spray dynamics and combustion characteristics. If the upstream pressure of the

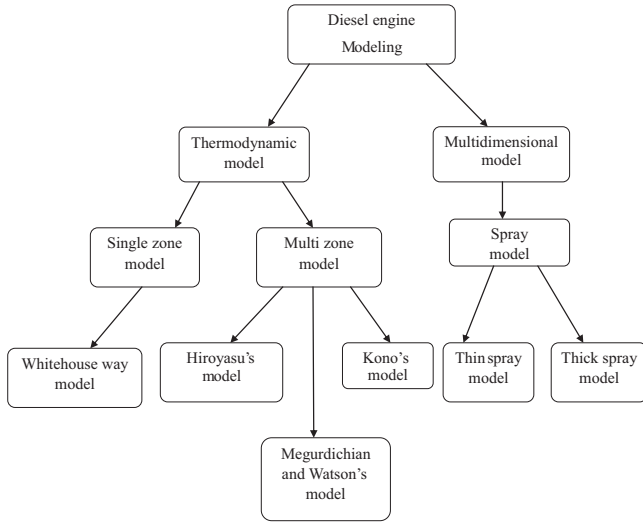


Fig. 1. Classification of diesel engine model.

Table 1

Mass flow rate equation for flow through exhaust valve.

Sl. no.	Mass flow rate equation	Critical condition
1.	$\frac{dm_e}{d\phi} = \frac{1}{6\eta} \mu_e F_e \frac{P}{\sqrt{RT}} \left(\frac{2^{1/(k-1)}}{k+1} \sqrt{\frac{2k}{k+1}} \right)$	$\frac{P_e}{P} \leq \frac{2^{k/(k-1)}}{k+1} \dots$ Supercritical flow
2.	$\frac{dm_e}{d\phi} = \frac{1}{6\eta} \mu_e F_e \frac{P}{\sqrt{RT}} \sqrt{\frac{2k}{k-1} \left(\frac{P_e^{2/k}}{P^{2/k}} - \frac{P_e^{(k+1)/k}}{P^{(k+1)/k}} \right)}$	$\frac{P_e}{P} \geq \frac{2^{k/(k-1)}}{k+1} \dots$ Subcritical flow

injector nozzle is known and assumed that flow through the nozzle is incompressible, one dimensional and quasi-steady, then the mass flow rate of fuel injected inside the cylinder through the nozzle is given by [2]

$$m = C_d A_n \sqrt{2\rho_l \Delta P} \quad (1)$$

In this type of mass flow rate, the intake and exhaust tanks (submodel) are treated as plenums with known temperatures and pressures. Earlier these models do not provide any information whether the flow is subcritical or supercritical at the inlet or outlet. They can be solved with the help of conservation of mass equation: in order to calculate the mass flow rate the equation is given by [15]

$$m = A_e P_1 \sqrt{\frac{\phi_1}{R_1 T_1}} \quad (2)$$

$$\phi_1 = \frac{2\gamma}{\gamma-1} \left[\left(\frac{P_2^{2/\gamma}}{P_1^{2/\gamma}} \right) - \left(\frac{P_2^{(\gamma+1)/\gamma}}{P_1^{(\gamma+1)/\gamma}} \right) \right] \quad (3)$$

These equations are further modified by taking into account the critical behavior of the fluid at intake manifold and exhaust manifold. The intake process is assumed as a subcritical flow and the intake flow rate is given as [16]

$$\frac{dm_s}{d\phi} = \frac{1}{6\eta} \mu_s F_s \sqrt{\left[\frac{2k_s}{k_s-1} \left(\frac{P_s^{2/k_s}}{P_s^{2/k_s}} - \frac{P_s^{(k_s+1)/k_s}}{P_s^{(k_s+1)/k_s}} \right) \right]} \quad (4)$$

During the exhaust process, the flow at outlet valve is considered as a supercritical flow due to higher pressure difference between cylinder and exhaust port. When the pressure at the outlet valve decreases, then the behavior of flow changes to subcritical flow. The calculation equation is given in Table 1.

2.2. Combustion submodel

Combustion model determines the rate of combustion. Whitehouse and Way [17] proposed a semi-empirical combustion model for the calculation of rate of combustion. The fuel is injected inside the cylinder in the liquid form with conical jets and forming the burning zone. However, before the fuel has to be burned it should be first heated, evaporated as well as mixed with sufficient amount of air entrained from the air zone through diffusion. This prepared fuel is ready for the chemical process and may be burned according to the rate governed by a chemical kinetics equation [18]. For the calculation of preparation rate the equation used is given as

$$P_r = K m_{finj}^{1-x} m_{fup}^x P_{O_2}^m \quad (5)$$

This expression was based on the assumption that the rate of preparation is proportional to the surface area of all droplets having uniform diameter, while Spalding [19] suggested that the rate of reaction is proportional to the droplets non-uniform diameter rather than uniform diameter. In order to compensate the non-uniform droplets diameter distribution exponent makes allowances for that fact. The last term in Eq. (5) shows the effect of oxygen availability on mixing to find out the reaction rate, for that purpose Arrhenius expression is used.

$$R = \frac{K P_{O_2}}{N \sqrt{T}} e^{-E_{red}/T} \int_0^\phi (P-R) d\phi \quad (6)$$

The combustion is further divided into two parts as diffusion and premixed combustion.

2.2.1. Diffusion and premixed combustion

Diesel combustion is mainly considered as diffusion combustion however it consist of premixed and diffusion phase, controlled by a fuel–air mixing process. Premixed phase of combustion occurs before the start of diffusion combustion. It plays a significant role in combustion process. Premixed combustion greatly influenced by the engine speed, load and injection process, mainly the quantity of fuel injected in cylinder during the ignition delay. The diffusion phase is governed by the turbulent mixing of air and fuel. The in-cylinder turbulence resulting from air motion and also fuel jet induced turbulence, which is predominant in modern high pressure injection system is used in modern engine [20–22].

In the recent years different burnt rate approaches are developed for premixed as well as diffusion combustion. Firstly, Vibe formula [23] was proposed for gasoline engines with totally premixed cylinder charge. This Vibe formula is also applicable for diesel engine and widely used for the diesel engine combustion modeling. This formula has only few drawbacks that it do not taking into account the consideration of injection rate. Another empirical approach was proposed by Schreiner [24] that includes the entire heat release history for combustion from polygonal sections followed by a hyperbolic function for the burn-out phase.

Austen and Lyn [25] described the individual burn rate as mixing controlled process by dividing the injected fuel in a number of packages. This work is further extended by Constien [26] who used a multizone approach for droplet evaporation, formation and mixing and explained it in detail. The burn rate formulation proposed by Hohlbaum [27] using the polygonal-hyperbolic burn rate history was further extended by a spray submodel based on the fact of gas jet theory. Weissner and Boulouchos [28] firstly described the diffusion combustion as a single stage mixing controlled process. Barba [29] carried out this formulation by adding a premixed combustion part and also considered the pilot injection.

2.3. Fuel spray submodel

2.3.1. Break up time calculation

For the calculation of break-up time, Hiroyasu equation [13] has been most commonly used. In the quasi-dimensional combustion model of diesel engine modeling which is based on the theory of phase-divided spray mixing model, it is considered that the fuel droplets subjected to atomization period, gasification period and eventually become gaseous after completion of break up time. The break up time is calculated according to Im and Huh [15] is given as

$$t_b = 28.65 \frac{\rho_l d_o}{\sqrt{\rho_a \Delta p}} \quad (7)$$

Reitz and Diwakar [30,31] included droplet break up for dense spray model calculations. They used KIVA-2 software code for two breakup regimes: (i) bag break up (ii) stripping break up. They shows that the droplet break up has strong influence of the spray penetration, vaporization and mixing in high pressure sprays. The size of spray droplets are controlled by coalescence and break up. They also include that droplet break up dominates in hollow-cone sprays because coalescences are minimized by expanding the spray geometry. Reitz and Diwakar [31] concluded that injected droplets having a diameter equal to the nozzle exit diameter. For the validation of computed length, droplet size, spray penetration and droplet velocity data compared with the available measured data in high pressure spray.

2.3.2. Droplet diameter after break up

In theory of combustion it is assumed that droplet after break up having the same initial diameter which is equal to the Sauter Mean Diameter (SMD) having neglecting droplets size distribution and the details of the atomization process. The following Eqs. (8)–(10) which are commonly used for the calculation of SMD in multizone models are given by Hiroyasu et al. [32] to compensate the variation of droplet size from one fuel parcel to the next allowance is made depending on the operating condition [33].

$$\frac{d_{32}^{LS}}{d_n} = 4.12 \text{Re}_i^{0.12} \text{We}_i^{-0.75} \left(\frac{\mu_l^{0.54}}{\mu_a^{0.54}} \right) \left(\frac{\rho_l^{0.18}}{\rho_a^{0.18}} \right) \quad (8)$$

$$\frac{d_{32}^{HS}}{d_n} = 0.38 \text{Re}_i^{0.25} \text{We}_i^{-0.32} \left(\frac{\mu_l^{0.37}}{\mu_a^{0.37}} \right) \left(\frac{\rho_l^{0.47}}{\rho_a^{0.47}} \right) \quad (9)$$

$$\frac{d_{32}}{d_n} = \text{MAX} \left(\frac{d_{32}^{LS}}{d_n}, \frac{d_{32}^{HS}}{d_n} \right) \quad (10)$$

Ingebo [34] developed a new theory for liquid jet breakups and shows that water jets in swirling and non-swirling flows, based on the acceleration waves. A correlation was developed for the ratio between the orifice diameter and SMD, and it can be expressed as

$$\frac{d_{inj}}{\text{SMD}} = C(W_E \text{Re})^{1/4} \quad (11)$$

Eq. (11) obtained is compared with the results of aerodynamics theory of liquid jet break up proposed by Reitz and Bracco [35] which predicts that SMD of liquid droplet is given by

$$\text{SMD} = B \times \frac{4\pi\sigma \times 3}{\rho U_{inj}^2 \times 2} \quad (12)$$

2.3.3. Fuel spray dynamics

In case of multidimensional models entire combustion chamber is taken as the computational domain and the fuel spray

is divided into a number of zones only for multizone model. Each zone control volume is treated as an open system where mass and energy equations are solved for individual zone.

In order to avoid the computational efficiency in case of multidimensional model, multizone model describe better the spray penetration with the help of empirical correlations instead of solving the full momentum equation. By the implementation of this method quasi-dimensional model provides the fastest and non-expensive means of generating the spatial information required to predict pollutant emission.

Since the multizone model based on empirical correlations to study the spray evolution, the fidelity of the spray penetration model is extremely important for accuracy. For accurate prediction of spray penetration Hiroyasu and Arai [36] proposed the following correlations before and after break up. Hiroyasu and Arai [36] correlation used is listed as follows:

$$S = 0.39 \sqrt{\frac{2\Delta p}{\rho_c}}, \quad 0 \leq t \leq t_b \quad (13)$$

$$S = 2.95 \sqrt{\frac{\Delta p}{\rho_a}} \sqrt{d_0 t}, \quad t_b \leq t \quad (14)$$

These correlations have been widely implemented in multizone models by different researchers [37–40]. These equations are valid only if the fuel elements are on the spray centerline. If the fuel elements in the radial direction away from the centerline then the equation changes to

$$X_r = X \exp[-4.403 \times 10^{-3}(L-1)^2] \quad (15)$$

where L ($=2, 3, 4, 5, \dots$), denotes the number of fuel elements injected per injection interval.

2.4. Ignition delay period

Ignition delay period is defined as the time interval between the actual dynamic injection point and ignition. The ignition delay period correlated to the cylinder pressure and temperature through the following semi-empirical equation given as [41].

$$t_d = a_1 P_m^{a_3} e^{a_2/t_m} \quad (16)$$

Ikegami et al. [42] and Tsao et al. [43] determined the induction period of diesel sprays in a rapid compression machine and reciprocating engine. Gerrish and Ayer [44], Spadaccini [45], Walsh and Cheng [46] and Scharnweber and Hoppie [47] concluded that ignition delay period decreases by the preheating of fuel before injection. Parker et al. [48] studied the effects of preheating of both the fuel and compressed air in a constant volume bomb to supercritical temperatures of pure n-dodecane which shows that ignition delay period can be expressed as

$$t_d = A \times e^{(T_a/T)} \quad (17)$$

Parker et al. [48] shows that preheating of the fuel before injection has a significant role in shortening of ignition delay period by diminishing the vaporizing and mixing times and concluded that induction period is insensitive to the combustion chamber pressure.

Hardenberg and Hase [49] proposed an empirical formula for the direct injection diesel engines to predict accurately ignition delay as a function of the fuel characteristics like cetane number, cylinder pressure, and temperature. Dent and Mehta [50] shows that result of this formula carried out good agreement with experimental data over a wide range of engine conditions. However, the pressure and temperature used in their correlation are identified as the corresponding conditions, when the ignition delay period starts at the end of TDC and can be estimated by

Table 2

Heat transfer coefficient correlation given by different authors [2].

S. No.	Author name	Heat transfer coefficient equations
1.	Eichelberg	$h_{ce} = 7.8 \times 10^{-11} \times up^{0.333} \times p^{0.5} \times T^{0.5}$
2.	Hohenberg	$h_{ch} = c_1 \times V^{0.8} \times p^{0.8} \times T^{-0.4} \times (up^{0.333} + c_2)^{0.8}$ $c_1 = 13 \times 10^{-3}$, $c_2 = 1.4$
3.	Woschni	$h_{cw} = 3.26 \times 10^{-3} \times D^{-0.2} \times p^{0.8} \times T^{-0.55} \times up^{0.8}$

using a polytropic model for the compression stroke. Belardini et al. [51] included that ignition delay time is a function of the compression ratio, rpm and swirl in direct injection diesel engines. It has also been concluded that there is no such correlation that fits experimental data. More fundamental equation proposed by Hardenberg and Hase [49] to calculate the ignition delay period is written as

$$t_d = \frac{n}{6} \times (0.36 + 0.22S_p) \exp\left(E_A\left(\frac{1}{RT} - \frac{1}{17190}\right) + \left(\frac{21.2}{P-12.4}\right)^{0.63}\right) \quad (18)$$

Considering the effect of change of pressure and temperature in combustion zone, the following condition is specified [52]:

$$t_{ig} = \int_0^{t_i} \frac{1}{t} d\phi, \quad t_{ig} \geq 1 \quad (19)$$

Wu [53] studied the effect of engine speed on the ignition delay period and concluded that as the engine speed is increased fuel burning rate in the premixed combustion phase decreased which cause increases in the ignition delay period. Wu also added that there is no correlation available to find the direct relation between ignition delay and premixed burning rate.

2.5. Heat transfer submodels

The heat transfer correlations of Annand [54] (including both the convective and radiations terms) Hohenberg, Woschni, Nussle and Eichelberg have been most commonly used for the calculation of instantaneous average heat transfer coefficients. Keribar and Morel [55] proposed exceptional model for the heat transfer calculation which includes the heat transfer through cylinder wall as well taking into consideration the heat transfer through cylinder head, piston crown, cylinder liner and valves. From the transient heat flux measurement in diesel engine it is concluded that due to spatial non-uniformities of the fluid flow and combustion cause different temperature histories at different point in the cylinder head [56].

Further study has been carried out for the heat transfer through engine to coolant and found that 20–35% of the fuel energy is transferred to coolant [57]. Primary heat transfer mechanism takes place through convection from the cylinder gases to the surrounding areas. Also heat transfer due to radiation is taken into consideration because temperature inside the cylinder during combustion is very much higher. Heat transfer through convection is given by Newton law of cooling:

$$\frac{dQ}{dt} = h_c A_c (T_{cyl} - T_{wall}) \quad (20)$$

The convection heat transfer coefficient (h_c) can be calculated by using different empirical approaches such as Woschni, Annand, Hohenberg and Eichelberg. Annand's formula has been found to be more fundamental equation which can be used to calculate the rate of heat transfer. This equation seems to be more fundamental than other alternative formulae available in the

Table 3

Calculation of rate constant [74].

Reaction	$K_{i,r}$ (cm ³ /mol s)	Author
1	$1.8 \times 10^4 \times \exp(-38,400/T)$ $0.544 \times 10^4 \times T^{0.1} \times \exp(-38,020/T)$ $0.76 \times 10^4 \times \exp(-38,000/T)$	Baulch et al. (1991) GRI-MECH 3.0 (2000) Heywood [2]
2.	$6.4 \times 10^9 \times \exp(-3150/T)$ $9.0 \times 10^9 \times \exp(-3280/T)$ $1.48 \times 10^8 \times T^{1.5} \times \exp(-2860/T)$	Baulch et al. (1991) GRI-MECH 3.0 (2000) Pattas (1973)
3.	6.4×10^{13} $3.36 \times 10^{13} \times \exp(-195/T)$ 4.1×10^{13}	Baulch et al. (1991) GRI-MECH 3.0 (2000) Heywood [2]

literature. This equation considers net heat transfer as the summation of both radiative and convective heat transfer rate. The net heat transfer is given by [58]

$$\frac{dQ}{dt} = a \frac{\lambda_g}{d} (Re^b) (T_w - T_g) + c (T_w^4 - T_g^4) \quad (21)$$

The total heat transfer in the two zones at each angle step is distributed in proportion to their kilo moles and absolute temperatures [59]. The heat transfer coefficient correlations given by different authors have been given in Table 2.

2.6. Pollutant formation

Basically nitrogen oxide and soot formation are two major pollutants from diesel engine emissions. Nitrogen oxide and particulate matter emissions from diesel engines are increasing rapidly due to usage of high speed engines. Due to the advantage of direct injection diesel engine leads research to minimize the emission aspect of high speed engines. The main challenging job for the designing of diesel engine is the reduction of NOx and soot simultaneously. So, a lot of research has been carried out on design of combustion and fuel injection system to minimize the pollutant emission. In order to control these emissions proper combination is required between combustion chamber configurations, fuel injection system nozzle diameter and optimum fuel injection timing.

For the objective of calculating the mass of combustion products of each zone, the complete chemical equilibrium system proposed by Vickland et al. [60] is used. It is considered that at any instant of time for each zone 11 species are present. These species are O₂, N₂, CO₂, H₂O, H, H₂, N, NO, O, OH, CO. By using this scheme a set of 11 equations is formed, by which the concentration of each zone's (11 species) has been obtained. By solving these equations, mass of fuel burned, volume temperature and mass of air entrained in each zone has been obtained [61]. Chemical equilibrium based upon the assumption, so it cannot correctly predict the concentration of NO and this drawback is overcome by chemical kinetics formation scheme proposed by Lavoie et al. [62].

Besides that a lot of work has been carried out on the property of diesel fuel to see the effect on combustion and exhaust emission of variable fuel property. To reduce the effect of acid rain, sulfur content in the diesel fuel has been reduced. Other fuel properties which are related to the improvement of engine performance and emissions include cetane number, density of fuel, viscosity, distillation temperature, oxygen and aromatic content has also been studied by different researchers [63–68].

Nakatani et al. [69] used the diesel particulate NO_x reduction (DPNR) catalyst and found that reduction in the NOx and particulates matter simultaneously. It has been noticed that more

than 80% of NO_x and PM has been reduced. Hosoya et al. [70] proposed model with selective catalytic convertor and diesel particulate filter (DPF) to reduce the NO_x and particulate matter and reported that by using selective catalytic reduction (SCR) NO_x emissions reduced by 72%. The above used model with the combination of DPF has been used and found a significant change in the reduction of particulate matter upto 93%.

NO_x is strongly affected by higher temperature inside the combustion chamber during the premixed and diffusion combustion. By lowering the combustion temperature inside the cylinder leads to reduction of NO_x emission but in other hand lowering temperature causes reduction of thermal efficiency which is not desirable. Supercharging strongly affect the combustion and reduces the injection rate which results in reduction of NO_x emission. Uchida et al. [71] studied the effect of supercharging and concluded that favorable result are obtained in the terms of fuel consumption and exhaust emission.

The extension of Zeldovich's model with the inclusion of OH [72] scheme is generally accepted as a very successful method for predicting NO concentration. The value of temperature, volume and equilibrium concentration for each zone is known and by using these values the concentration of NO in each zone has been calculated by integrating the equation referring to the change of NO concentration at any instant of time. By the addition of NO concentration for all zones at a certain time, the total [NO] concentration inside the combustion chamber [73] has been obtained. Chemical reactions are given below:



Rate of reaction k_1 , k_2 , k_3 are calculated with the help of Table 3.

2.7. Soot formation submodel

Soot is basically produced when nondiluted spray produces fuel rich vapor regions and undergoes chemical reaction. It has also been formed on liquid film along the cylinder walls. Flower [75] shows that with the increase in pressure volumetric rate of soot formation in laminar diffusion flames increases. Rah et al. [76] proposed a correlation of NO and soot formation with the ignition of liquid fuel droplet. It also included that soot formation can be suppressed by delaying the ignition, vaporizing as much as fuel possible prior to the ignition. Rah et al. [76] also proposed a possible method of controlling the NO_x and soot emission by using of low oxygen concentration in oxidation to delay ignition and high fuel–air ratio to reduce NO_x.

Uyehara [77] shows that in diesel engine maximum amount of the soot occurs in the temperature range of 2000–4000 K. It also shows that less than this temperature, soot formation rate is negligible. Kagami et al. [78] studies the effect of fuel Cetane number, viscosity and distillation range on the performance of gaseous and smoke emission, knocking, fuel consumption, startability and cold performance of diesel engine. The result shows that the fuel with low Cetane number produces higher emission and also shows that the fuel consumption is high as compared to fuel which is having very high Cetane number.

Tateishi et al. [79] proposed a new combustion model for indirect diesel injection (IDI) diesel engines and show that this model reduces the fuel consumption, emission and noise. Engine noise is due to rise in very high peak pressure at the early stage of combustion, when there rapid heat release rate has been

occurred. Sinnamon and Cole [80] used sampling to study the pollutant emission from a prechamber stratified charge engine. They concluded that prechamber induces turbulence which helps to increases the fuel–air mixing rates and reduces the combustion interval. They also show that with the increment in the degree of stratification beyond a certain limit resulting in higher formation of NO and CO emission even if lean air–fuel ratio has been used.

Anna [81] proposed a thermodynamic model to predict the soot formation and oxidation rate of diesel engine. This model has been based upon the one step chemical reaction and D² law and also included droplet interference and forced convection effect. It has been assumed that during the vaporization and combustion processes liquid fuel droplets maintain their spherical symmetry throughout.

Hiroyasu et al. [13] proposed a model for the calculations of net soot formation. According to this model, there is a soot formation oxidation rate, which consider the available fuel mass and oxygen of each zone (by including its partial pressure) respectively. So, net soot formation rate is calculated by subtracting the soot oxidation rate from the formation one. By integrating each zone separately over time, the total value of soot formation inside the combustion chamber is calculated by adding the corresponding values for all the zones. Hiroyasu et al. [13] proposed soot formation model is implemented in multizone models to calculate the soot formation. The soot formation rate is calculated by assuming that vaporize fuel having a first-order reaction which is given by the equation:

$$\frac{dm_s}{dt} = m_{sf} - m_{sc} \quad (25)$$

$$m_{sf} = A_f m_{fg} p^{0.5} e^{-(E_{sf}/RT)} \quad (26)$$

$$m_{sc} = A_c m_s \frac{P_{O_2}}{P} p^{1.8} e^{-(E_{sc}/RT)} \quad (27)$$

Lipkea and DeJoode [82] modified the previous model and formed a new set of equation to calculate the net soot formation. According to this model soot formation and soot oxidation rate is calculated as follows:

$$\frac{dm_{sf}}{dt} = A_{sf} dm_{f}^{0.8} p^{0.5} e^{-(E_{sf}/R_{mol}T)} \quad (28)$$

$$\frac{dm_{sc}}{dt} = A_{sc} dm_{sn} \left(\frac{p_{O_2}}{p} \right) p^n e^{-(E_{sc}/R_{mol}T)} \quad (29)$$

Therefore, the net soot formation is expressed as follows:

$$\frac{dm_s}{dt} = \frac{dm_{sf}}{dt} - \frac{dm_{sc}}{dt} \quad (30)$$

The net soot formation rate is proposed by Khan–Hiroyasu–Belardini expression and soot oxidation rate given by Nagle–Strickland Constable expression is given as [73]:

$$\frac{dm_s}{dt} = \frac{dm_{sf}}{dt} - \frac{dm_{so}}{dt} \quad (31)$$

$$\frac{dm_{sf}}{dt} = A_f e^{-(T_f/T)} m_{fv} \quad (32)$$

$$\frac{dm_{so}}{dt} = \frac{6M_c}{\rho_s D_s} m_s R_{so} \quad (33)$$

Single zone, two zone and multizone models are proposed by the different author as listed in Table 4.

3. Results and discussions

In this literature review different modeling approach is used to understand the behavior of diesel engine modeling and on the

Table 4

Comparative study of different models of CI engine.

Author name/country and year	Model used	Engine spe. (B/S/CR) rpm	Parameter studied	HTC/exp val.	Submodel used	Results
Ziarati/UK (1990) [83]	Single zone model	(215/241/11/) na	Delay Period, droplet penetration	Annand/ yes	Combustion, heat transfer and spray model	Model is capable to run under heavy fuel and diesel fuel Shows good agreement of cylinder pressure and temperature with experimental result.
Ishida/Japan (1994) [84]	Two zone model	(100/105/ na) 3500	NO _x emission, pressure, temperature and ignition delay	na/yes	Heat release model, Ignition delay model, NO _x emission model	NO _x emission is reduced by retarding the time by decreasing the maximum combustion temperature and pressure in expansion stroke. NO _x reduces by using small nozzle diameter is caused by decreasing the combustion pressure.
Rakopolous/Greece (1994) [85]	Multi zone model	(86/80/18.5/) 1200,1500,3100	Insulation effect on performance and exhaust emission on diesel engine	K-EModel/ no	Fuel spray, evaporation, ignition delay, heat transfer, chemical combustion model	No remarkable change in engine efficiency has been seen but increases in the exhaust enthalpy helps to improve overall engine efficiency by using power turbine Increment in the NO and soot formation occurs by the insulation effect that is not desirable.
Belardini/Italy (1996) [86]	3-D model	(199/95/17/)na	NO _x and soot formation, heat	na/yes	NO _x , soot formation, ignition delay,	The model over predicts both acetylene and soot volume fraction. However, it is noted that better results can be obtained with a careful optimization of the model constants.
Yong/Pohang (2000) [15]	Multi-zone model	(123/155/17.1/) 1200,1400,1600,1800	IMEP, pressure traces, NO _x and soot emissions, fuel injection timing,swirl ratio	Woschni/ yes	Intake and exhaust manifold, NO _x , Ignition delay, Air entrainment, In cylinder flow effect and Fuel evaporation model	In cylinder flow model is combined with Hiroyasu model both model shows results consistent with the general operating characteristics of a DI diesel engine. The calculated imep, pressure traces, brake specific NO _x and soot emissions studied by the present model shows good agreement with the test bed measurements at full and part load conditions for a range of the engine speeds.
Jung/Michigan (2001) [87]	Quasi – dimensional multi-zone model	(130/160/15)2100	Pressure, temperature, ignition delay, combustion, NO and soot formation	Assian– Heywood/ yes	Ignition delay model, heat transfer model, air entrainment model, spray evaporation model	Extended Zeldovich mechanism accurately predicted the NO and soot formation. At least five zones are recommended to determine the NO and soot in radial direction. Modified Hiroyasu correlation for spray tip penetration show good agreement with experimental data in a range of injection pressure.
Papagiannakis/Greece (2004) [88]	Single zone model	(85.73/82.55/17.6) 1000–3000	Pressure, heat release, brake specific fuel consumption, NO _x , CO, HC and soot emission	na/no	HCCI model, heat transfer model, pollutant formation model	Exhaust emission and performance of engine study have been carried out at different speeds and loads for diesel and dual fuel (combination of diesel and gaseous fuel). Dual fuel combustion process has lower peak cylinder temperature in comparison to conventional diesel. NO _x and soot emission is low and HC and CO emission is high in dual fuel operation compared to normal diesel operation.
Rakopolous/Greece (2004)[58]	Two zone model	(82/88.90/na)4500	The growth of the fuel spray zone, jet mixing, C–H–O system	Annand/ yes	Fuel Preparation,combustion Model, NO _x , Soot Formation model	Two zone models proves to very efficient for the determination of engine performance and exhaust emission by concerning the effect of two major parameter of load and injection timing. Theoretical result show good agreement with exp. value.
Zheng/China (2005)[89]	Multi-dimensional model	(95/115/20) 1200,1600	Pressure, temperature, ignition timing, natural	na/yes		Injection time, natural gas composition and initial temperature have a significant effect on ignition,

Table 4 (continued)

Author name/country and year	Model used	Engine spe. (B/S/CR) rpm	Parameter studied	HTC/exp val.	Submodel used	Results
			gas composition, NO emission		Combustion model, turbulence model, mixture formation model, No formation model	combustion and emission. Increased amount of ethane in natural gas provide advance in ignition and increment in NO emission. Auto-ignition of natural gas occurs at 1300 K of mixture temperature and NO emission reduce when fuel injection timing delay.
Tauzia/France (2006)[90]	Phenomenological Model	(123.8/165/16.5) 1900–3000	Premixed combustion, pressure, temperature	na/yes/cfd-kiva 3v	Premixed combustion model, Ignition delay model	Model studied at injection timing -16° to $+12^\circ$ ATDC shows good agreement with experimental and CFD analysis from a quantitative and qualitative point of view for ignition delay and in-cylinder pressure evolution during combustion.
Xingcai/China (2006) [91]	Multi-zone model	(98/105/18.5)1800	IMEP, thermal efficiency, pressure, heat release rate, ignition timing, emission characteristics	na/yes	HCCI combustion model, pollutant model	Energy input, ignition timing, maximum gas pressure is deteriorated with increase of ethanol addition. For all fuels, CO emission is very high at 1.5–2.5 bar of engine load. When IMEP is larger than 3 bar ignition timing lies in -5° CA ATDC-TDC.
Chmela/Austria (2007) [92]	Zero Dimensional ROHR Model	na	Premixed combustion based on Arrhenius and Mangussen equation.	na/no	Ignition delay, Premixed and diffusion combustion, Reaction Rate combustion Model	An improved model for diffusion combustion is presented which shows a sequential approach. Ignition delay and premixed combustion model solved by Arrhenius and Magnussen approach shows better description of the effects of considerably transient ROI shapes by using a more detailed consideration of the processes in the fuel jet.
Sundarapandian/India (2007) [93]	Multizone model	(87.5/110/17)1500	Heat release, work done, and harmful pollutant such as HC, CO, NO _x and smoke.	Annand/yes	Combustion and heat release, heat transfer, engine performance like specific fuel consumption, brake thermal efficiency	Heat release is reduced by 4–8% for vegetable oil esters compared to diesel fuel. Pressure of vegetable oils esters are reduced about 4%, 5% and 7% respectively for Jatropa, mahua and neem oil ester compared to diesel. But the negative impact has been seen on thermal efficiency reduced by 3%, 4% and 5% for Jatropa, mahua and neem oil ester compared to diesel. CO reduced by 19% for Jatropa and 16% for the mahua and neem oil ester compared to diesel.
Machrafi/France (2008) [94]	Single zone model	(82.55/114.5/4–14)na	Heat release ratio, equivalence ratio, ignition delay, compression ratio	na/yes	Combustion model ignition delay model, heat released model	Heat release increase with increase in equivalence ratio which is affected by ignition delay. Compression ratio provides advancing in ignition delay and lower residual gas fraction. Variation of inlet temperature is directly affected the ignition delay but heat release distribution did not affected the ignition delays.
Sahin/Turkey (2008) [95]	Multi-zone model	na	Details of fuel spray, heat transfer, swirl model, engine performance	Annand/yes	Heat transfer, combustion model, spray model, NO emission model,	Indicated thermal efficiency at 2500 rpm by present model is 0.4420 and Li model is 0.43 shows that in result only 3% of error occurs. Equivalence ratio changes between 1.086 to 1.1.49 while actual ration like 0.650–0.80 so model is not adequate at low equivalence ratio.

Semin/Malaysia (2008) [96]	Single zone model	(86/70/na)200–4000	MEP, mean piston speed, specific power output, sfc intake valve mach index.	na/no	Parametric model –MEP, SFC, power output, mean piston speed.	From engine modeling it is concluded that highest brake power is 4.314 kW and indicator power is 5.725 kW occurs at 3000 rpm. The engine modeling brake torque maximum is 14.3662 Nm and indicated torque is 18.743 Nm occurs at 2800 rpm. At 2800 rpm, the engine model has shown the lowest value of the BSFC and the indicated specific fuel consumption.
Garcia/Spain (2009) [97]	Single zone model	(95/100/19) 1500–2400	Pressure, fuel specific consumption, start of combustion, NO _x , CO, HC and soot emission	na/no	Combustion model, pollutant model, HCCI combustion model	HCCI combustion process provides low NO _x and soot emission than the diesel mode. HCCI with exhaust gas recirculation (EGR) has a great impact on combustion and emission. When angular speed increases, start of combustion that affected by inlet temperature at constant EGR rate, decrease.
Huang/China (2009)[98]	Multi-dimensional CFD model, single zone model	(115/115/17)1400	Pressure profiles, combustion process, HC and CO emission	na/yes	Turbulence model, combustion model, mixture formation model, HCCI combustion	HCCI combustion process does not take place simultaneously in combustion chamber core zone. High temperature reaction occurs in vicinity of piston surface. Unburned fuel and CO increase when Di-methyl ether (DME) equivalence ratio decreases. Pressure profile of multi-dimensional CFD model is more accurate than the single zone model because turbulence flow and wall heat transfer is measured.
Kannan/India (2009) [99]	Single zone mode	(87.5/110/17.5)1500	Heat release rate, pressure, brake thermal efficiency, bsfc NO formation	Hohenberg/ yes	Ignition delay model, heat transfer model, pollutant emission model.	From simulation result it is concluded that 18% and 21.5% of reduction in NO is achieved with 10% and 20% dilution of diesel with water emulsion respectively. The brake thermal efficiency increases as reported by Abu – Zaid by 3.5% by increasing the water emulsion by 20% over the use of diesel for the engine speed range studied.
Komninos/Greece (2009)[100]	Multizone model	(120.65/140/17)na	Mass transfer effect on emission i.e. unburned HC and CO emission,	Annand/ yes	Heat transfer as well as pollutant formation model	Neglecting mass transfer prior to main heat release would result in a severe underestimation of the HC accumulated in the crevices during combustion (60% for the case Studied). Neglecting mass transfer during combustion and expansion would result to and underestimation of the final HC amount by at least 14% for the case studied.
Kuleshov/Moscow (2009) [101]	Multizone Model (RK-model)	(88/85/17.6)1800	Heat release inside the cylinder and NO _x formation, inlet manifold pressure and EGR rate	Woschni/ yes	combustion model, fuel spray model, gas exchange model, ignition delay model	The RK-model accounts for drop size interaction of free sprays with swirl effect, spray and wall impingement, evolution of near-wall flow formed by spray, hit of fuel on cylinder head surface and swirl intensity on heat release rate. This model helps in designing of piston bowl shape, numbers of injector holes, diameters and directions in match with swirl intensity to control emission and fuel consumption.
Liu/China (2009) [102]	Two Zone Model	(102/120/18:1) 800–2000	Mass distribution, heat transfer, mass exchange between zones, heat transfer in porous medium and studied the effect of PM on performance	Woschni/ na	Heat transfer model, mass exchange model, porous medium model, chemical kinematics	The compression ratio of 13 is great enough for the auto-ignition in the porous medium engine, which is not so crucial like in the HCCI engine. For the same intake pressure of 1 atm, the pressure in the PM engine is relatively lower than that of a traditional engine due to the voids in PM, which lowers the ignition delay and higher engine output. Due to higher average temperature in PM engine NO emission is higher at excess air ratio of 1.6.

Table 4 (continued)

Author name/country and year	Model used	Engine spe. (B/S/CR) rpm	Parameter studied	HTC/exp val.	Submodel used	Results
Dhuchakallaya/UK (2010) [103]	Spray model	na	Combustion, spray dynamics and ignition delay	na/na	Combustion model, Ignition model	Higher lift of length cause the increases of air entrainment in the premixed combustion zone resulting in high reaction rate. Simulation results show good agreement with experimental results at time of 4 ms of start of injection.
Gogoi/India (2010) [104]	Single zone model	(87.5/110/14–20)600–2000	Engine performance- IMPEP, BTE comparative study of diesel with biodiesel blends	Annand/no	Heat transfer, ignition delay model, gas exchange model	Maximum brake power occurs at design speed and further increases of speed decrease brake power. For CR of 17.5 the maximum peak power occurred at 1500 rpm for B20 and B40 blends while for B60 it occurs at 1400 rpm. Increased brake power was observed for B40 and B60 blends as compared to diesel fuel. Blends B20, B40 and B60 shows an increase in thermal efficiency due to increases in break power as compared to diesel engine.
Prasad/India (2010) [105]	Two Zone Model	(11/127/16)1000–1500	Pressure, heat release, heat transfer and performance characteristics –SFC, BTE	Annand/yes	Preparation rate and reaction rate model for the calculation of heat transfer rate.	The cylinder pressure for low heat rejection biodiesel is lowers than LHR diesel about 1% and higher about 4% and 2.5% for TC biodiesel and TC diesel. Brake thermal efficiency of LHR biodiesel engine is lower than that of LHR diesel and higher than TC biodiesel and TC diesel operation this is because of lower calorific value of biodiesel as compared to diesel fuel.
Qi/China (2010) [106]	Quasi-dimensional two zone model	(135/150/17) 1500	Diesel engine performance- sfc, effect of air entrainment and spray mixing model	Newton/yes	Spray mixing, combustion model, ignition delay period, heat transfer, pollutant formation, intake and exhaust flow model	Simulation result shows good accordance with experimental result proves the validation of phase divided spray mixing model. The relative error between simulation and experimental result for the specific fuel consumption and NO emission occur to be 2.8% and 9.1%. By using this model computational time is 36 s to analyze engine working process.
Rakopolous/Greece (2010) [107]	Quasi-dimensional	(85.73/82.55/17.61) 500–2500	Cylinder flow field and gas temperature distribution.	na/CFD model	heat transfer, fuel injection rate, spray penetration, evaporation, combustion and pollutant formation	Both quasi-dimensional and CFD model are compared for the different piston bowl geometry changing from (d/D) from 64% to 44% at different rotational speed. It is concluded that both models predict the quite similar cylinder pressure and temperature, traces whole closed cycle of the engine.
Shankra/India (2010) [108]	Multidimensional model (CFD model)	(130/150/15.5:1) 2000	CFD model proposed to study the effect of intake pressure, fuel injection on the performance of DI engine	Eckert/yes	CFD based—combustion and ignitions model, turbulence model, NO _x and soot formation and droplet breakup model,	It is observed that by advancing injection time cause results in the increases pressure, temperature heat release rate, cumulative heat release and NO _x emissions by 6.88%. If we reverse the trend then NO _x emissions by 6.85%. Higher NO _x (15.03% and 58.69% at 1.21 bar and 1.71 bar respectively) and lower soot emission (8.82% and 51.47% at 1.21 bar and 1.71 bar) concluded that optimum injection time and intake pressure is 12° bTDC and 1.21 bar.
Shi/USA (2010) [109]	Multidimensional model	(137.16/165.1/16.1) 1300	Pressure, injection timing, specific fuel consumption, soot formation, NO _x , CO, UHC emission	na/yes	Adaptive multi-grid chemistry model, combustion model	At high load, high volatility fuel as gasoline and E10 have less sensitivity to fuel reactivity. So these are better for fuel economy. For cleaner combustion, gasoline fuels are more efficient than normal diesel fuel.

Normal diesel is affected by first injection amount but gasoline fuel is affected by second injection timing.

Som/USA (2010) [110] na	Single zone model	(50/200/na) na/yes	Spray and combustion characteristic, fuel penetration, temperature contours, flame index		KH breakup model, spray and combustion model, aerodynamically induced breakup model, soot formation	-KH-ACT model have better performance of parameters such as injection pressure, ambient density and fuel temperature with vapour penetration for evaporating spray. -The inclusion of turbulence and cavitations enhances the primary breakup process, decreases in liquid penetration and increases in radial dispersion. -Enhancing spray breakup provides ignition length and flame stabilization near nozzle exit.
Reiter/USA (2011) [111]	Multi-zone model	(106/127/17) 1000	Pressure, heat release rate, engine break specific fuel consumption, soot formation	na/ no	Ignition delay model, combustion and heat release model, pollutant formation model, soot formation model	In dual fuel engine, ignition delay is longer due to increased ammonia and resulting peak combustion pressure is low. BSFC of diesel is high below 40% of diesel fuel energy. NO emission is low by using less than 40% ammonia in dual fuel compared 100% of diesel.
Boretti/USA (2012)[112]	Multi-zone model	(131/158/18)1900	Cumulative heat release, pressure, heat release, pollutant emission	na/no	Combustion model with jet ignition and diesel ignition, stochastic reactor model (SRM), soot model	Diesel injection during compression and expansion to build up the pressure are best options to develop a pressure profile. Thermal efficiency of diesel injection and hydrogen jet ignition combustion models is 10% larger than the diesel at high loads.
Komninos/Greece (2012) [113]	Single zone, multi-zone and multidimensional model	na	Chemical kinematics modeling, different reaction mechanisms for biofuel combustion simulation	na	HCCI combustion model, direct injection HCCI, fully premixed HCCI, emission model	Present the effect of various configurations in single zone model such as negative valve overlap, heavy EGR, fuel reforming on biofuel HCCI combustion. Study the multi-zone models for mixture thermal and fuel stratification which provide better and more realistic estimates on combustion duration, peak combustion pressure and emissions formation. Multi-dimensional models provide higher spatial resolution of the combustion chamber than the multi-zone model.
Visakhamoorthy/Canada (2012) [114]	Multi-Zone model	(72/73.6/22) 1500	Pressure, heat release rate, Emissions, predicted NO _x levels	Yes/ yes	HCCI engine model, mixture composition model, pollutant model	The model represents good quality HRR and pressure prediction curves after calibration. When engine operating point is close to misfire limit, model is unable to handle cyclic variability i.e. to predict the pressure. Predicted NO _x emission increase with small increase in cylinder temperature.

HTC—heat transfer correlation, B—Bore of cylinder, Spe.—Specification, Exp.—Experimental, S—Stoke length, Val.—Validation, CR—Compression ratio.

basis of these modeling approach, following result has been obtained and discussed below:

1. Insulation effect on the cylinder wall is studied by the multi-zone model and it is concluded that by the increasing the degree of insulation causes increment in the NO_x emission and simultaneously increases soot formation. This increase in emission and soot formation is not admirable because of negative impact on the environment. However, the engine efficiency is improved by providing more insulation on the cylinder wall. So, it is suggested that degree of insulation should be properly selected.
2. Rate of heat release (ROHR) model proves very effective to accurately predict the different instantaneous parameter which controls the diffusion combustion and also it takes very less computational time.
3. Single zone approach by using the water diesel combustion emulsion has been successfully modeled to predict the engine performance parameters. It has been found out that with the 20% increases in the water emulsion brake thermal efficiency (BTE) of the engine increases by 3.5% which is significant improvement for diesel engine. Similarly the NO_x emission reduced from 21% to 18.5% by increasing the water emulsion from 10% to 20%.
4. CFD study is carried out for the detailed analysis on the multizone model to study the effect of intake pressure, injection timing on the NO_x and soot formation. From the analysis it is concluded that with the increase in the intake pressure NO_x emission increases while soot formation rate decreases. So, from the three intakes pressure range 1.01, 1.21 and 1.71 bar the 1.21 bar gives more desirable optimum result which compensate both type of emissions. Similarly out of 16, 12 and 8 bTDC injection timing the 12 CAD found to be providing more optimum result of pollutant emission.
5. Ignition delay model is studied at different cetane numbers and variable speed by using Hardenberg equation and concluded that with the increases in the engine speed the ignition delay period increase while with the increase of the cetane number.

4. Conclusion

In this present article single zone, multizone, and multi-dimensional models of diesel engine combustion has been reviewed. Single zone model has been found to more effective tool for immediate prediction of engine parameter but case by case adjustment of the wiebe function parameter is required. Theses wiebe function parameter deals with engine geometry and operating condition. Multizone model account for air entrainment and inhomogeneities of the mixture and overcome the drawback of single zone model. Multi-dimensional models account for both engine geometry temporal as well as spatial variation of the flow field. These accurately predict the spray behavior and fuel spray dynamics model. These model included the CFD analysis which accurately predict the combustion behavior and help to reduce the pollutant emission at great extent make diesel engine more reliable and fewer impact on the environment.

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